

# A note on the Karhunen-Loève expansions for infinite-dimensional Bayesian inverse problems

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## Abstract

In this note, we consider the truncated Karhunen-Loève expansion for approximating solutions to infinite dimensional inverse problems. We show that, under certain conditions, the bound of the error between a solution and its finite-dimensional approximation can be estimated without the knowledge of the solution.

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## 1 Introduction

Nonparametric inverse problems have applications in many scientific or engineering problems, ranging from geophysical tomography [2] to medical imaging [6]. In such problems the unknown that we want to determine is of infinite-dimension, for example, a function of space or time.

Identifying the unknown is usually cast as an optimization problem that needs to be solved numerically. Infinite-dimensional problems can not be solved directly with standard numerical techniques. A common practice is to first approximate the unknown with a finite-dimensional parameter, and then solve the resulting finite-dimensional problem numerically. In particular, when the inverse problem is treated in a Bayesian framework, the Karhunen-Loève (K-L) expansion ([10], Chapter 11) can be used to construct such a finite-dimensional

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approximation. In the K-L method, the unknown is represented by a finite expansion of the eigenfunctions of the covariance operator of the prior measure.

The K-L method has been long used to reduce the dimensionality in practical problems [9,7,8]; however, the use of it is never rigorously justified to the best of my knowledge. To be specific, it is unclear whether a fixed-dimensional representation can well approximate the solutions of the problem. In this note, we address the problem by proving that, if  $u$  is a solution to the inverse problem defined as a minimizer to Eq (2), the error bound between  $u$  and its finite K-L approximation can be estimated without the knowledge of  $u$ .

## 2 Problem setup

We consider the inverse problems in a Bayesian framework (see [11] for a comprehensive overview of the Bayesian methods for infinite-dimensional inverse problems). We assume the state space  $X$  is a separable Hilbert space with inner product  $\langle \cdot, \cdot \rangle_X$ . Our goal is to estimate  $u \in X$  from some data  $y$ . The Bayes' formula in this setting should be interpreted as providing the Radon-Nikodym derivative between the posterior measure  $\mu$  and the prior measure  $\mu_0$  [3,5]:

$$\frac{d\mu}{d\mu_0}(u) = \exp(-\Phi(u)), \quad (1)$$

where  $\exp(-\Phi(u))$  is the likelihood function. A typical example is to assume that the unknown  $u$  is mapped to the data  $y$  via a forward model  $y = G(u) + \zeta$ , where  $G : X \rightarrow R^d$  and  $\zeta$  is a  $d$ -dimensional Gaussian noise with mean zero and covariance  $C$ . In this case  $\Phi(u) = |C^{-\frac{1}{2}}(Gu - y)|_2^2$ .

Next we assume a Gaussian prior is used. Namely we let  $\mu_0$  be a zero-mean Gaussian measure defined on  $X$  with covariance operator  $Q$ . Note that  $Q$  is symmetric positive and of trace class.  $E = Q^{\frac{1}{2}}(X)$  is a Hilbert space with inner product

$$\langle \cdot, \cdot \rangle_E = \langle Q^{-\frac{1}{2}} \cdot, Q^{-\frac{1}{2}} \cdot \rangle_X,$$

which is known as the Cameron-Martin space associated with measure  $\mu_0$ . Often we are only interested in a point estimate of  $u$ , rather than the posterior measure  $\mu$  itself. To this end, as is shown in [3,5], the maximum a posterior (MAP) estimator of  $u$  can be defined as the minimizers of the Onsager-Machlup functional over  $E$ :

$$\min_{u \in E} I(u) := \Phi(u) + \|u\|_E^2, \quad (2)$$

where  $\|u\|_E^2 = \langle u, u \rangle_E$ . Note that Eq. (2) can also be understood as a classic inverse problem where the cost function  $\Phi(\cdot)$  is minimized with a Tikhonov regularization in the Hilbert space  $E$  [1].

### 3 Karhunen-Loève representation

Note that solving Eq. (2) directly involves inverting the operator  $Q$ , which can be rather challenging in practice. Alternatively, one can use substitution  $u = Q^{\frac{1}{2}}x$  and rewrite Eq. (2) as

$$\min_{x \in X} J(x) := \Phi(Q^{\frac{1}{2}}x) + \|x\|_X^2. \quad (3)$$

The following proposition states the equivalence of the two optimization problems.

**Proposition 3.1** *If  $x$  minimizes  $J(x)$  over  $X$ ,  $u = Q^{\frac{1}{2}}x$  minimizes  $I(u)$  over  $E$ , and if  $u$  minimizes  $I(u)$  over  $E$ ,  $x = Q^{-\frac{1}{2}}u \in X$  minimizes  $J(x)$  over  $X$ .*

*Proof.* We prove the proposition by contradiction. First it is easy to verify that, for any  $x \in X$  and  $u \in E$  satisfying  $u = Q^{\frac{1}{2}}x$ , we have  $I(u) = J(x)$ . Let  $x$  be a minimizer  $J(\cdot)$  over  $X$ , and assume  $u = Q^{\frac{1}{2}}x$  is not a minimizer of  $I(\cdot)$  over  $E$ . Namely, there exists an  $u' \in E$  such that  $I(u') < I(u)$ . It follows directly that  $x' = Q^{-\frac{1}{2}}u' \in X$  and  $J(x') < J(x)$ , which contradicts that  $x$  is a minimizer of  $J$  over  $X$ . Thus we have proved the first part of the proposition. The second part can be proved by following the same argument.  $\square$

Now we introduce the K-L expansion to reduce the dimensionality of Eq. (3). We start with the following lemma ([4], Chapter 1):

**Lemma 3.2** *There exists a complete orthonormal basis  $\{e_k\}_{k \in \mathbb{N}}$  on  $X$  and a sequence of non-negative numbers  $\{\lambda_k\}_{k \in \mathbb{N}}$  such that  $Qe_k = \lambda_k e_k$  and  $\sum_{k=1}^{\infty} \lambda_k < \infty$ , i.e.,  $\{e_k\}_{k \in \mathbb{N}}$  and  $\{\lambda_k\}_{k \in \mathbb{N}}$  being the eigenfunctions and eigenvalues of  $Q$  respectively.*

The basic idea of the K-L method is to solve the optimization problem in a finite-dimensional subspace of  $X$ :

$$\min_{x \in X_n} J(x) := \Phi(Q^{\frac{1}{2}}x) + \|x\|_X^2, \quad (4)$$

where  $X_n$  be the space spanned by  $\{e_k\}_{k=1}^n$  for a given  $n \in \mathbb{N}$ . In numerical implementation Eq. (4) can be recast as

$$\min_{(\xi_1, \dots, \xi_n) \in \mathbb{R}^n} \Phi\left(\sum_{k=1}^n \xi_k \sqrt{\lambda_k} e_k\right) + \sum_{k=1}^n \xi_k^2 \quad (5)$$

which is the usual K-L representation. As is mentioned earlier, a critical question here is whether the finite subspace  $X_n$  can provide good approximation to the solutions of Eq. (3). Our main results regarding this problem are presented in the following theorem:

**Theorem 3.3** Suppose  $\Phi(u)$  is locally Lipschitz continuous, i.e., for every  $r > 0$ , there exists a constant  $L_r > 0$  such that for all  $z_1, z_2 \in X$  with  $\|z_1\|_X, \|z_2\|_X < r$ , we have

$$|\Phi(z_1) - \Phi(z_2)| < L_r \|z_1 - z_2\|_X.$$

Let  $\{e_k\}_{k \in \mathbb{N}}$  and  $\{\lambda_k\}_{k \in \mathbb{N}}$  be the eigenfunctions and eigenvalues of  $Q$  as defined in Lemma 3.2. There exists a constant  $L > 0$  such that, for any  $x \in \arg \min_{x \in X} J(x)$ , we have

$$\|x - x_n\|_X < L\sqrt{\lambda_n^*}$$

where  $x_n = \sum_{k=1}^n \langle x, e_k \rangle_X e_k$ , and  $\lambda_n^* = \max_{k > n} \lambda_k$ .

*Proof.* Let  $x \in X$  be a minimizer of Eq. (3). Since  $\{e_k\}$  is a complete orthonormal basis for  $X$ ,  $x$  can be written as

$$x = \sum_{k=1}^{\infty} \xi_k e_k,$$

where  $\xi_k = \langle x, e_k \rangle_X$ . Let

$$x_n = \sum_{k=1}^n \xi_k e_k.$$

As  $x$  is a minimizer of  $J(\cdot)$ , take  $r = \Phi(0) + 1$  and so we have  $J(x) < r$ , which implies that  $\|x_n\|_X \leq \|x\|_X < r$ .  $Q^{\frac{1}{2}}$  is bounded, and so we have  $\|Q^{\frac{1}{2}}x_n\|_X, \|Q^{\frac{1}{2}}x\|_X < \|Q^{\frac{1}{2}}\|r$ . Now recall that  $\Phi(\cdot)$  is locally Lipschitz continuous, and so there exists a constant  $L > 0$  such that

$$|\Phi(Q^{\frac{1}{2}}x) - \Phi(Q^{\frac{1}{2}}x_n)| < L\|Q^{\frac{1}{2}}x - Q^{\frac{1}{2}}x_n\|_X.$$

Since  $x$  minimizes  $J(\cdot)$ , we have  $J(x) \leq J(x_n)$  which implies

$$\begin{aligned} \|x - x_n\|_X^2 &\leq |\Phi(Q^{\frac{1}{2}}x) - \Phi(Q^{\frac{1}{2}}x_n)| < L\|Q^{\frac{1}{2}}x - Q^{\frac{1}{2}}x_n\|_X \\ &= L\langle x - x_n, Q(x - x_n) \rangle_X^{\frac{1}{2}} = L\langle \sum_{k=n+1}^{\infty} \xi_k e_k, \sum_{k=n+1}^{\infty} \xi_k \lambda_k e_k \rangle_X^{\frac{1}{2}} \\ &= L\sqrt{\sum_{k=n+1}^{\infty} \lambda_k \xi_k^2} \leq L\sqrt{\lambda_n^*} \|x - x_n\|_X. \end{aligned}$$

It then follows immediately that

$$\|x - x_n\|_X \leq L\sqrt{\lambda_n^*}.$$

□

Certainly we also want to know if the minimizer of the original problem (2) is well approximated by the K-L expansion. To this end, we have the following corollary, which is a direct consequence of Theorem 3.3:

**Corollary 3.4** *Let  $u = Q^{\frac{1}{2}}x$  and  $u_n = Q^{\frac{1}{2}}x_n$ , and we have  $\|u - u_n\|_X < L\lambda_n^*$ .*

Another important question is that whether a solution to finite-dimensional problem (4) is a good approximation to that of the infinite-dimensional problem (3). We have the following results regarding this issue:

**Corollary 3.5** *Let  $x'_n \in \arg \min_{x \in X_n} J(x)$  and we have*

$$\min_{x \in X} J(x) \leq J(x'_n) \leq \min_{x \in X} J(x) + L^2 \lambda_n^*$$

The corollary follows directly from Theorem 3.3 and so proof is omitted.

## 4 Concluding remarks

We theoretically study the truncated K-L expansions for approximating the solutions of infinite-dimensional Bayesian inverse problems. We show that the error between a solution to the inverse problem and its projection on the chosen finite-dimensional space is bounded by the eigenvalues of the covariance operator of the prior.

## Acknowledgment

The work is supported by the NSFC under grant number 11301337.

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